Code Intercomparison Builds Confidence in Numerical Models for Geologic Disposal of CO_2

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ABSTRACT

Numerical simulators were exercised on a suite of test problems for CO_2 disposal in saline aquifers and depleting oil and gas reservoirs. Intercomparison of results reveals broad agreement in most areas, but also points out sensitivities to fluid properties and discretization approaches that need further study.

INTRODUCTION

Different kinds of subsurface reservoirs have been proposed for geologic disposal of greenhouse gases, including saline aquifers (brine formations), depleted or depleting oil and gas reservoirs, and coalbeds. Injection of greenhouse gases into such formations will give rise to complex coupled processes of fluid flow, mechanical and chemical changes, and heat transfer. Mathematical models and numerical simulation tools will play an important role in evaluating the feasibility of geologic disposal of CO_2, and in designing and monitoring CO_2 disposal operations. The models must accurately represent the major physical and chemical processes induced by injection of CO_2 into potential disposal reservoirs, such as miscible and immiscible displacement, partitioning of CO_2 among different fluid phases, chemical reactions, thermal effects, and geomechanical changes from increased pore pressures. It is essential to test and evaluate numerical simulation codes, to establish their ability to model these processes in a realistic and quantitative fashion. The code intercomparison study reported here is a first step in this direction.

APPROACH

The present study was initiated and coordinated by Lawrence Berkeley National Laboratory [1]. It was decided to include only brine formation, oil, and gas reservoir problems, for which well-developed simulation capabilities are available. Coalbed simulators are less mature and are the subject of a separate

address basic processes in different potential disposal reservoirs. Hence it was felt that problem specifications should be kept relatively simple. Most problems are for 1-D homogeneous media, although a heterogeneous 2-D problem was also included. Problems with more complex and realistic features, such as 3-D heterogeneous flows systems, will be addressed in future studies.

The initial set has eight test problems which are summarized in Table 1. Full specifications are available in [1]. Participation in the study was solicited by mail and e-mail, as well as through web postings [1] and a conference presentation [3]. Space discretization (gridding) and fluid property data were not prescribed, and associated effects are evaluated as part of the intercomparison. All participants worked with their own funding, and used codes available to them. A two-day workshop was held in Berkeley in October 2001, at which preliminary results were compared and detailed specifications for results to be submitted were agreed upon. The proposers of each of the test problems served as coordinators and communicated with the various participating groups in obtaining and collating results. Here we present a brief summary and evaluation of results for problems 3 through 8. The gas reservoir problems (1 and 2) are discussed in a separate paper at this conference[4]; a more extensive report with full intercomparisons of all simulation results is in preparation.

TABLE 1
TEST PROBLEMS FOR CODE INTERCOMPARISON STUDY

problem		storage reservoir	property and process features
#1	mixing of stably stratified gases	gas reservoirs	PVT data, gas advection and diffusion
#2	advective-diffusive mixing due to lateral density gradient	gas reservoirs	PVT data, gas advection and diffusion
#3	radial flow from a CO_2 injection well	saline aquifers	PVT data, two-phase flow, phase partitioning
#4	CO_2 discharge along a fault zone	saline aquifers	PVT data, two-phase flow, phase partitioning, buoyancy effects
#5	mineral trapping in a glauconitic sandstone aquifer	saline aquifers	chemical reactions between rocks and fluids
#6	hydromechanical responses during CO_2 injection into an aquifer-caprock system	saline aquifers	coupling between fluid flow and rock deformation
#7	CO_2 injection into a 2-D layered brine formation	saline aquifers	PVT data, two-phase flow, heterogeneous formations
#8	CO_2-oil displacement and phase behavior	oil reservoirs	PVT data, phase behavior, two-phase flow

RESULTS

Problem 3: Radial Flow from a CO_2 Injection Well

This is a basic CO_2 injection problem that addresses two-phase flow of CO_2 and (saline) water for simplified flow geometry and medium properties. CO_2 is injected at a rate of 100 kg/s into a brine aquifer that is assumed infinite, homogeneous, and isotropic. Initial conditions include temperature: 45 ˚C; pressure: 120 bar; and salinity: 15 % NaCl by weight; as a problem variation, a case without salinity was to be run also. Gravity and inertial effects are neglected, and flow is assumed 1-D radial (line source). Under the conditions stated the problem has a similarity solution where dependence on radial distance R and time t occurs only through the similarity variable $\eta = R^2/t$ [5]. Results of interest include pressures, gas saturations, dissolved CO_2 mass fractions, and "solid saturations" (fraction of pore volume with precipitated salt).

Comparison of thermophysical property data showed good agreement for density and viscosity of the aqueous phase (< 1 %), while larger differences of up to 10 % for density and up to 20 % for viscosity were

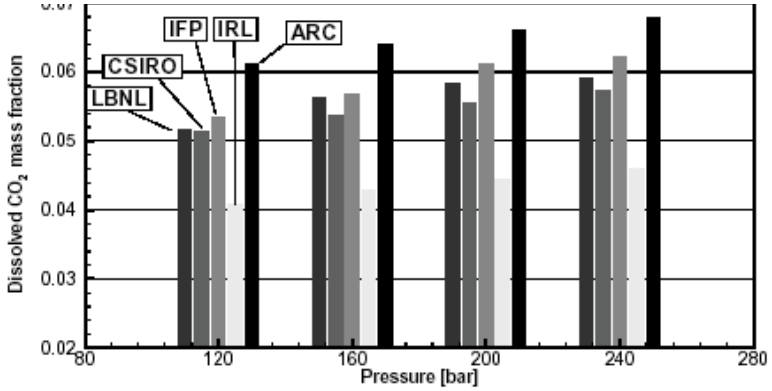


Figure 1: CO_2 mass fraction in the aqueous phase at T = 45 ˚C at different pressures (bar); no salinity. (For initials, see affiliation list of authors.)

The similarity property was checked by plotting results for different R and t as a function of the similarity variable. With minor exceptions the results from all groups were found to satisfy this invariance. Fig. 2 shows simulated pressures and gas saturations from five groups for the case without salinity. Pressures agree within the specified comparison criterion of better than +/- 5 %. For gas saturations, the results from three groups that use different in-house versions of the TOUGH2 code (LBNL, IRL, and CSIRO) are practically identical, while larger discrepancies are noted with two groups whose simulators do not consider dry-out near the injection well. These results show explicitly the significance of the dry-out zone.

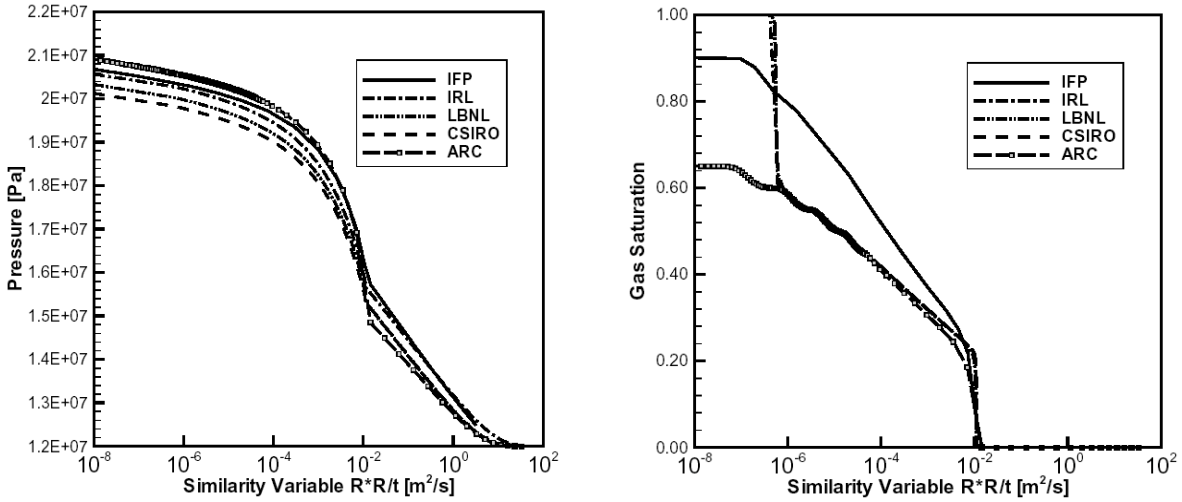
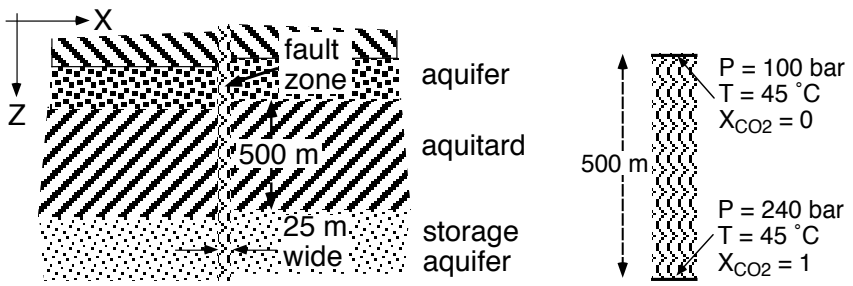


Figure 2: Simulated pressures and gas saturations as a function of the similarity variable; no salinity.

Problem 4: CO_2 Discharge Along a Fault Zone

This problem explores CO_2 loss from storage through a leaky fault, using a highly simplified 1-D linear flow geometry [6]. It is envisioned that the storage aquifer is intersected by a vertical fault, which establishes a connection through an otherwise impermeable caprock to another aquifer 500 m above (Fig. 3a). This situation is idealized by assuming 1-D flow geometry and constant pressure boundary conditions as shown in Fig. 3b. Hydrogeologic parameters are similar to those of problem 3.



The CO_2 entering at the base of the fault displaces water upward. Two snapshots of the displacement front at times of 10^7 and $2x10^7$ seconds, respectively, are shown in Fig. 4a, while Fig. 4b gives the corresponding profiles of dissolved CO_2 concentrations. The LBNL, CSIRO, IRL, and LANL simulations agree in terms of frontal saturation and displacement profile, but differ with respect to how far the CO_2 displacement front has advanced. These differences are explained by differences in aqueous phase solubilities (Fig. 4b), with less CO_2 dissolution corresponding to a more advanced front. The LBNL calculation did not include a Poynting correction, hence overestimated CO_2 solubility. The IFP calculation shows significantly different saturations behind the front.

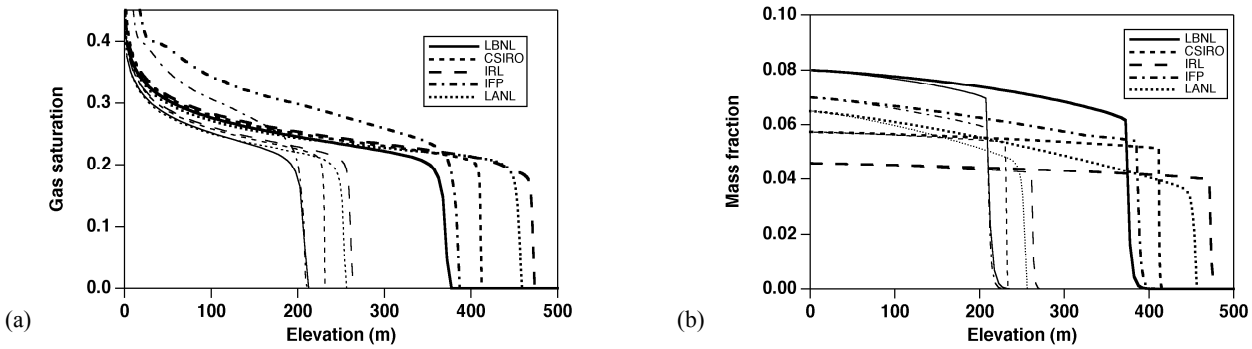


Figure 4: Gas saturations (a) and CO_2 mass fractions dissolved in the aqueous phase (b). Results after 10^7 seconds are shown as thin lines, results after $2x10^7$ seconds as heavy lines.

Problem 5: Mineral Trapping in a Glauconitic Sandstone Aquifer

This problem addresses geochemical effects of CO_2 injection into a glauconitic sandstone aquifer, and analyzes the impact of CO_2 immobilization through carbonate precipitation. Batch reaction modeling of the geochemical evolution of this aquifer is performed in the presence of CO_2 at a pressure of 260 bar. The problem is based on Gunter et al. [7] who modeled water-rock reactions when CO_2 is injected into a glauconitic sandstone aquifer in the Alberta Sedimentary Basin, Canada. The current modeling considered (1) equilibrium aqueous-aqueous and aqueous-gas reactions, (2) redox, (3) the presence of organic matter, (4) the kinetics of chemical interactions between the host-rock minerals and the aqueous phase, and (5) CO_2 solubility dependence on pressure, temperature and salinity of the system. Results include evolution of aqueous phase composition, and changes in mineral abundances.

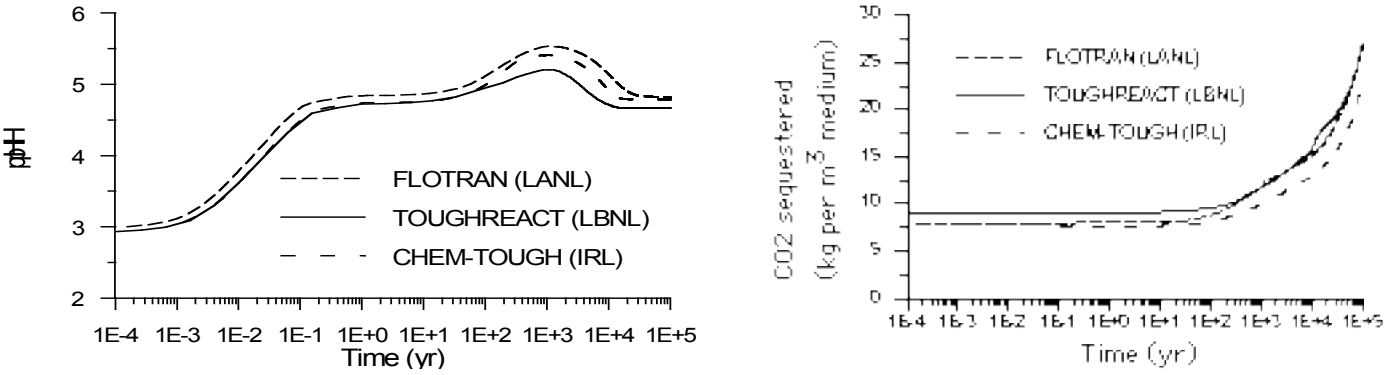


Figure 5: Simulated evolution of solution pH and total CO_2 sequestration.

Three groups studied this problem, LBNL using TOUGHREACT, LANL using FLOTRAN, and IRL using CHEM-TOUGH2. Fig. 5 shows reasonable agreement between their simulation results for solution pH and total CO_2 sequestration in aqueous and solid phases. Results for the temporal evolution of mineral abundances also show satisfactory agreement.

Problem 6: Hydromechanical Response of an Aquifer-Caprock System

At this time only LBNL has conducted simulations for this test case. Results are available in a recent

Problem 7: CO_2 Injection into a 2-D Layered Brine Formation

This test problem is patterned after the CO_2 injection project at the Sleipner Vest field in the Norwegian sector of the North Sea, and is intended to investigate the dominant physical processes associated with the injection of supercritical CO_2 into a layered medium. Significant simplifications have been made, the most important of which is the assumption of isothermal conditions (37 ˚C, the ambient temperature of the formation). CO_2 injection rates (1,000,000 tonnes per year), system geometry, and system permeabilities correspond approximately to those at Sleipner, although no attempt was made to represent details of the permeability structure within the host formation. Injection of the supercritical CO_2, which is less dense than the saline formation waters into which it is injected, causes it to rise through the formation. Its rate of ascent, however, is limited by the presence of four relatively low permeability shales. The top and bottom of the formation is assumed to be impermeable. The system is idealized as a two dimensional symmetric domain perpendicular to the horizontal injection well which has a screen length of 100 meters (Figure 6). A one meter thick section perpendicular to the horizontal well is considered.

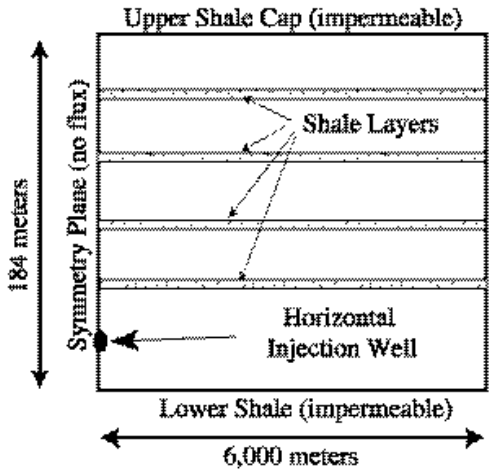


Figure 6: 2-D vertical section for CO_2 injection into the Utsira formation.

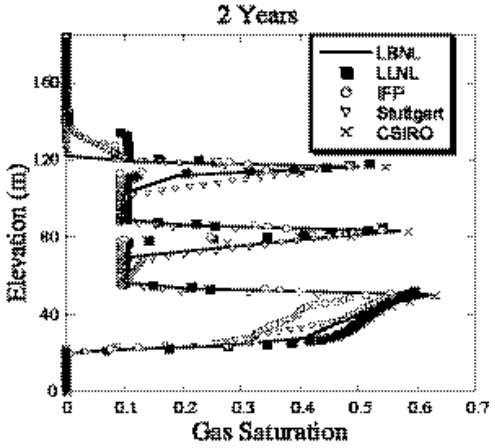


Figure 7: Simulated gas saturations.

Fig. 7 shows gas saturations after two years of simulation time along a vertical line at 500 m distance from the symmetry plane. Upflow of gas is impeded by the shale layers, leading to gas accumulation beneath the layers. Gas saturations obtained by the different groups are in reasonable agreement. No gas migration beyond the top shale layer has occurred at this time. Closer inspection and comparison suggests that differences in simulated results may arise from differences in aqueous solubility of CO2, and from different space discretization.

Problem 8: CO_2-Oil Displacement and Phase Behavior

This problem tests our ability to calculate the interplay of CO_2-oil phase behavior and multiphase flow. CO_2 is injected into an oil-containing homogeneous porous medium for two different initial pressures that lead to immiscible and near-miscible displacement, respectively. The oil consists of 10% CH_4, 20% C_4, and 70% C_{10} by mole. The different volatilities of the oil components cause chromatographic separation as fluid components partition between the CO_2-rich gas phase and the oil phase. Comparisons between numerical simulations evaluate the representation of multiphase flow, the description of miscibility and phase behavior in the presence of CO_2, the formulation of constitutive relations (such as density, viscosity, and CO_2 solubility), and the degree of dispersion in numerical solutions.

The problem is posed in a one-dimensional geometry so that direct comparison can be made to analytical solutions obtained with the method of characteristics (MOC). Results for gas saturations and CO_2 mole fractions in the gas phase are plotted in Fig. 8 for the near-miscible case.

Numerical solutions include results from a Stanford University research code that uses explicit time integration and two levels of space discretization (100 grid blocks - SU 100; 5000 grid blocks - SU 5000),

labeled ARC were obtained with the GEM code using 5000 grid blocks, while LANL used ECLIPSE 300 and 50 grid blocks. It is seen that discrepancies between analytical and numerical solutions decrease as grid resolution is increased, but even with 5000 grid blocks significant smearing of sharp fronts persists, emphasizing the strong sensitivity of the interplay between space resolution, phase behavior, and multiphase flow.

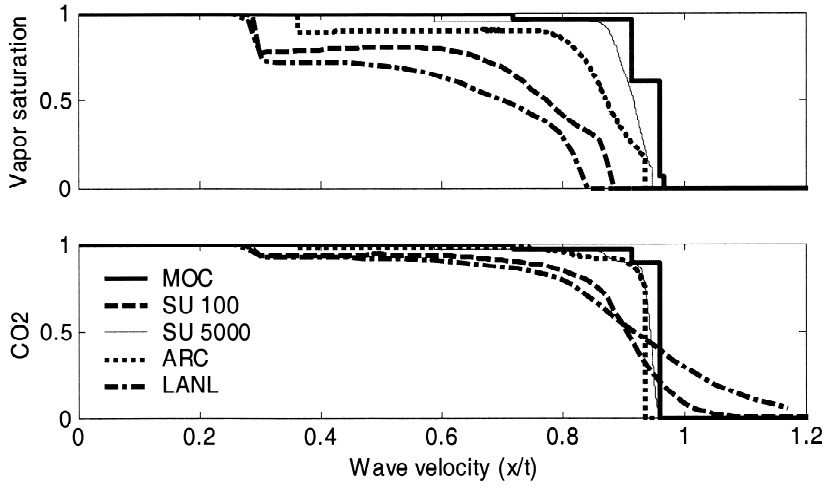


Figure 8: Gas saturations and CO_2 mole fractions in the gas phase for near-miscible oil displacement by CO_2.

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